ELECTRON-IMPACT EXCITATION OF INTERSTELLAR MOLECULES

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ABSTRACT

Electron-molecule collisions play a crucial role in astrophysical environments where the electron fraction is higher than about 10^{-5}, e.g. in the diffuse ISM, PDRs or comets. We present here a brief review of our recent R-matrix calculations of rate coefficients for electron-impact rotational excitation of interstellar molecules. Our major result is the prediction of emission lines from higher rotational states than previously assumed. Rate coefficients for transitions with $\Delta j > 1$ are indeed found to be significant and in some cases larger than those with $\Delta j = 1$, the only ones considered previously. This reflects the importance of short-range interactions which are ignored in the standard theories. Illustrative results are presented for CH^+, H_3^+ and H_2O.

Key words: Molecular data; molecular processes; ISM.

1. INTRODUCTION

Rate coefficients for the collisional excitation of interstellar molecules by electrons are crucial parameters for modelling the physical conditions of harsh molecular environments such as diffuse clouds, photodissociation regions, cometary comae, etc. In such environments, the observed intensities of molecular emission depend on a complex competition between radiative and collisional processes. A good knowledge of state-to-state collisional excitation rates is therefore necessary. As it has been generally not possible to obtain these parameters experimentally, theoretical estimates have proved very useful to astronomers. It is thus known that even at modest electron fractions, $n(e)/n(H_2) \approx 10^{-5}$ to 10^{-4}, electron collisions can dominate the molecular excitation because electron-impact collisional rates exceed that for excitation by the more abundant neutral partners (H, He and H_2) by typically 5 orders of magnitude. The reference methods for obtaining electron-impact excitation rates have been the Born and Coulomb-Born theories for, respectively, neutral and ionic targets [1,2]. Based on simple long-range approximations, these theories predict that only single jumps in vibrational or rotational quanta are allowed for polar species. Recent **R**-matrix *ab initio* studies have shown that this prediction is incorrect: the inclusion of short-range electron-molecule interactions can indeed change the molecular internal states by several quanta. As a result, transitions with $\Delta j > 1$ do have significant rates (see e.g. [3]). In this paper, sample results are presented for astronomically important molecules.

2. RESULTS

2.1. CH^+

CH^+ was the first ever molecular ion to be observed in the interstellar medium, via its optical spectrum. Observations of CH^+ have persistently given abundances greater than theoretical models: CH^+ has indeed chemical lifetimes that are inconsistent with large abundances. For such reactive species, collisional processes are crucial to interpret spectra. *ISO* observations of the planetary nebula NGC 7027 have, for the first time, recorded pure rotational spectra of CH^+ [4]. These observations were interpreted in terms of LTE with a rather low temperature (150 K) and a H_2 density as large as $5 \times 10^7 \mathrm{cm}^{-3}$. **R**-matrix calculations by Lim et al. [5] have shown that provided an electron fraction larger than 10^{-4} (warm PDR), electron collisions alone can explain the high level of CH^+ rotational excitation inferred from the line ratios observed by Cernicharo et al. [4].

2.2. H_3^+

H_3^+ is generally considered as a fundamental molecule of interstellar chemistry because it reacts efficiently with almost any neutral atom or molecule to initiate a complex network of ion-neutral reactions. Recent observations revealed the presence of H_3^+ in diffuse clouds [6]. The detection of H_3^+ in the diffuse interstellar medium was quite surprising because this

ion is thought to be destroyed rapidly by dissociative recombination with electrons. Our **R**-matrix calculations [7] have shown that electron-impact excitation is very efficient to pump the rotational levels of this ion: such collisions essentially conserve the K quantum number but can change J by up to three quanta. In particular, we have found that electrons could help to create and maintain the predicted population inversion between the $(J, K) = (4, 4)$ and $(3, 1)$ levels of H_3^+ [8].

2.3. H_2O

Water vapour has been detected in a great variety of astronomical objects using both spacecraft and Earth-based observations. The satellites *ISO*, *SWAS* and *ODIN* have revealed the ubiquity of water in the interstellar medium, from star-forming regions to envelopes of evolved stars. Electron-impact excitation of the water molecule has been widely studied, both experimentally and theoretically, for many years. As the comparison with experimental differential cross sections (DCS) is often the only reliable way for testing calculations, we have computed the elastic (rotationally summed) DCS for electron scattering from H_2O at electron energies investigated experimentally. In the figure below, our calculations [9] are compared with the recent experimental results of Cho et al. [10]. It can be noticed that our calculations reproduce the experimental data very well.

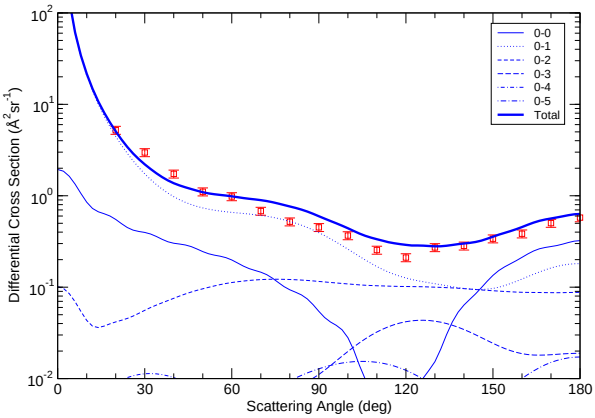

Figure 1. Elastic (rotationally summed) DCS of water at 4 eV. The squares are the experimental points from [10]. The present calculation is given by the thick solid line. Other lines denote partial state-to-state DCS.

As noted by Strelnitskij [12], electron collisions might contribute to the pumping of H_2O masers which are commonly observed in star-forming regions or active galactic nuclei. Use of our transition rates should help to assess and clarify the exact role of electrons in cosmic water masers. Finally, in the context of cometary comae where the electron fraction exceeds 10^{-3}, current models are based on overestimated H_2O-H_2O collisional rates. Our calculations have shown that electron collisions are expected to largely dominate the water excitation in such environments.

2.4. Conclusion

Rate coefficients for electron-impact excitation of interstellar molecules have been revisited in the context of **R**-matrix theory. Our calculations suggest that the role of such collisions have been underestimated in the astrophysical litterature: electrons are among the most efficient exciting species in harsh molecular environments.

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